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INTEGRATING EXPERIMENTATION, MODELING, AND VISUALIZATION THROUGH FULL-FIELD METHODS (PREPRINT)

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Recent research in which full-field techniques are used is presented. This work includes the study of deformation through modeling and experimentation both in the vicinity of material defects and in areas without defects. For the latter, nonlinear, full-field strain resulting from the heterogeneity of the material's microstructure can be studied, enabling the evaluation and calibration of advanced microstructural-deformation models to much greater extent than previously possible. Through the study of microstructural deformation near defects, the effect of microstructural variability on damage evolution can be better understood, leading to better understanding of the underlying physics of variability in damage evolution.

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Integrating Experimentation, Modeling, and Visualization through Full-field Methods

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ABSTRACT

Recent research in which full-field techniques are used is presented. This work includes the study of deformation through modeling and experimentation both in the vicinity of material defects and in areas without defects. For the latter, nonlinear, full-field strain resulting from the heterogeneity of the material's microstructure can be studied, enabling the evaluation and calibration of advanced microstructural-deformation models to much greater extent than previously possible. Through the study of microstructural deformation near defects, the effect of microstructural variability on damage evolution can be better understood, leading to better understanding of the underlying physics of variability in damage evolution.

Introduction

Evaluation and calibration of sophisticated, physics-based models are hampered by the relative paucity of data that is available through traditional test techniques. As an example, information available from a tension test typically consists of the applied load and strain averaged over a single area or the relative displacement change between two points of the specimen. This quantity of information may be sufficient for the simplest models, but more detailed physics-based models, which attempt to describe material behavior through understanding of the effect of material structure at various size scales, require a much greater amount of data. Modern physics-based constitutive models include parameters and state variables that control not only the nominal material stiffness, but effects of localized slip, strain gradients, anisotropic and cyclic hardening, orientation mismatch, dislocation density, and other relevant characteristics. Accordingly, these models require a great deal of detailed data, and in many cases may benefit from the availability of multiple data samples. The availability of detailed experimental measurements at the microstructural scale, harvested from essentially the same tests as engineers have used traditionally to obtain modulus, yield stress, strength and elongation, provides sufficient information to define and calibrate the more sophisticated material models now under development. This process leads to *verified* modeling and simulation, providing, in turn, a much better fundamental physical understanding of material behavior and the potential for extensive cost savings in the entire materials life cycle.

Modern experimental techniques offer great promise in acquiring such large data samples. In the case of the tension specimen, for example, full-field techniques can continuously determine the full two-dimensional and, in some cases, three-dimensional strain tensor for every point on the

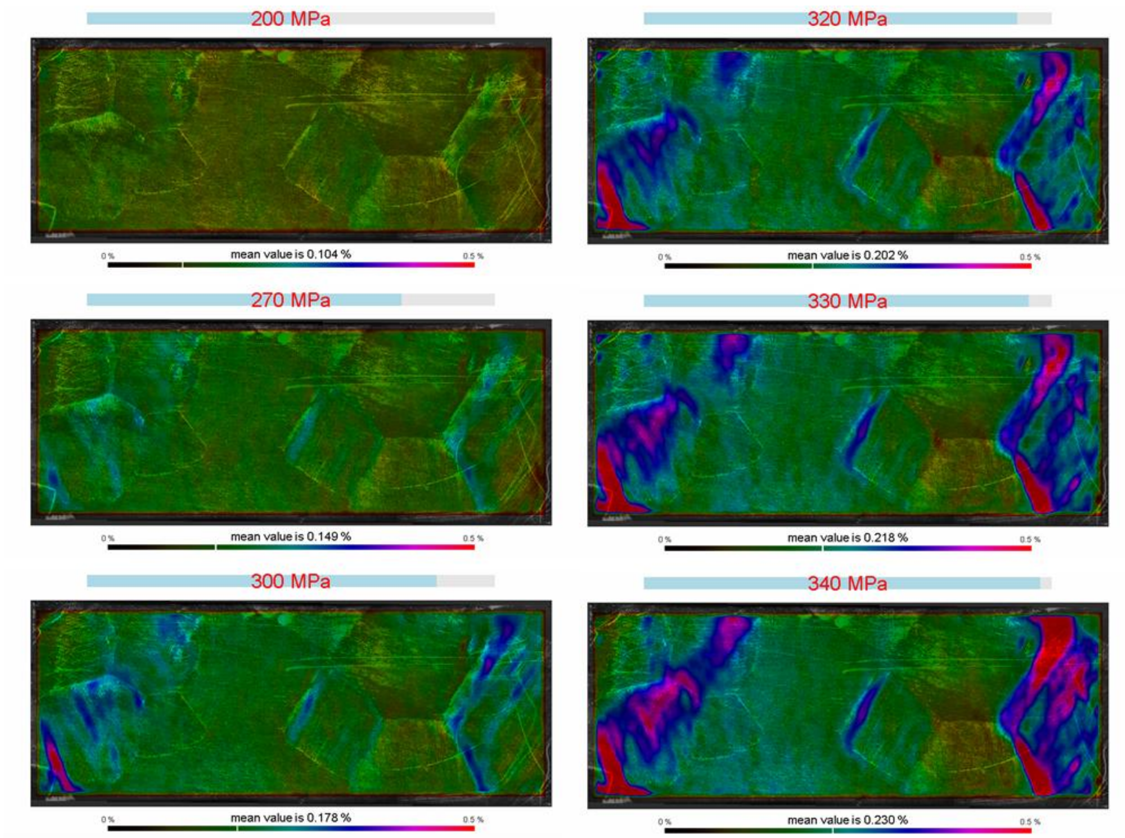

Figure 1. Full-field, in-plane, maximum principal stress in a fully lamellar titanium aluminide undergoing tensile loading. Field of view in larger dimension is approximately 5 mm. [1]

surface of the specimen's region of interest throughout the duration of the test. This observation can be accomplished at various size scales. The resulting information is vital in calibrating and evaluating modern models of general, nonlinear, material behavior. Figure 1 illustrates the ability of full-field techniques to measure the details of microstructural deformation. The ability to determine much lower strain levels compared with other techniques used in the past should be noted. The quantity of data collected through full-field techniques is so great as to be difficult to present in its entirety on the written page. Results such as those shown are available at all deformation states, enabling the very efficient evaluation and calibration of general, nonlinear models. This process supplies the vitally needed connection between microstructure and behavior mentioned above.

Much attention has been focused on integrating modeling and experiments, but the emphasis has typically been on model development. It is the author's contention that, in the materials-behavior area, modeling efforts are typically far ahead of our ability to judge the efficacy and practicality of those models. Therefore, more attention should be focused on efficient and sophisticated experimental methods at all size scales, fully integrated with a modeling effort. Also, the tools that enable correlation between results from experiments and from models are relatively unsophisticated and need much greater development.

Figure 2 illustrates the philosophy behind this new approach to modeling and experimental integration. In conventional experimentation, a series of tests are conducted, and very limited data are collected, generally only at the global scale. The example illustrated is a series of stress-strain plots from tension tests, but the same approach is typical of almost all materials-research experimentation, including fatigue, fatigue-crack growth, tribology, fracture toughness,

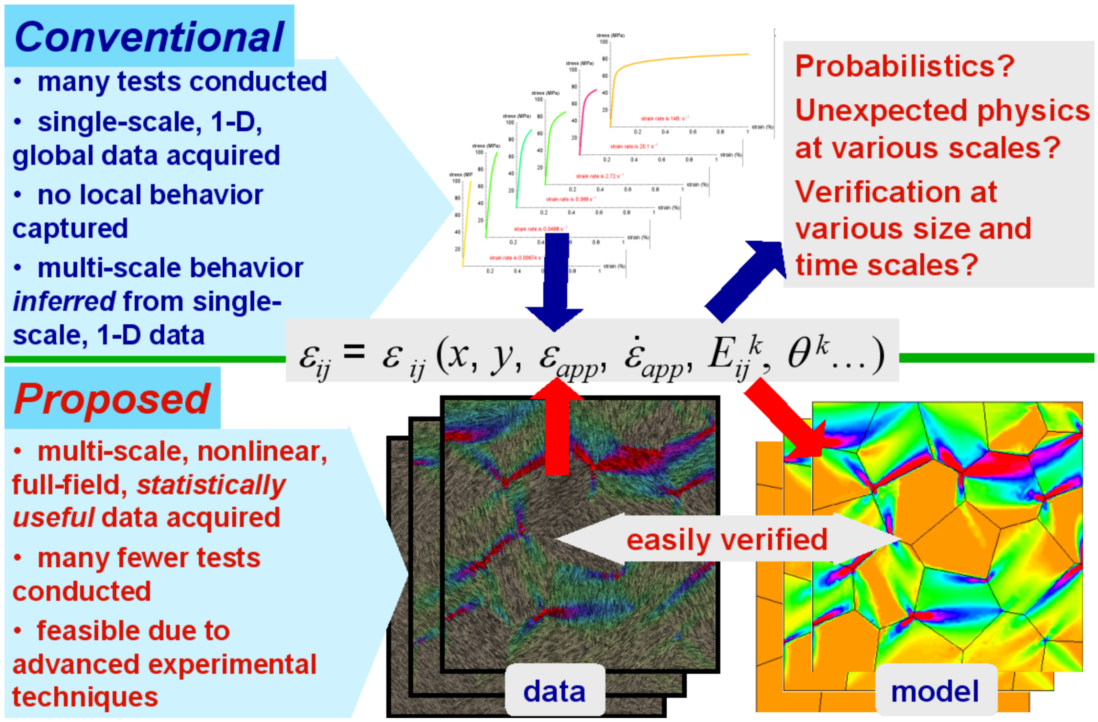

Figure 2. Comparison of conventional and advanced modeling/experimentation integration. [1]

and so on. In each case, an entire suite of expensive testing is necessary to acquire enough data to understand the effect of just a few parameters on the particular material behavior being studied. However, even with all of this testing, the study of probabilistic effects would require many more tests for statistically valid conclusions. Also, because only global data are acquired, unexpected physics at various scales will not be apparent, contributing to the lack of fidelity in any related multi-scale modeling effort. In contrast to this conventional approach, advanced, full-field experimental techniques enable a new approach, which is much more conducive to true modeling/experiment integration. This approach is schematically shown in the bottom illustration in Figure 2. Here, full-field data is collected, consisting of displacements (from which strains can be derived) in a solid's region-of-interest (ROI) while the solid undergoes various changes in loading conditions. These loading-condition changes can include time-dependent mechanical, thermal, or any other environmental changes which would induce a deformation-state change in the solid. By automatically scanning across a wide region of the solid, sufficient data can be collected for statistically valid study of the material-parameter distributions. Also, by repeatedly collecting data of the same ROI, general, nonlinear behavior can be studied in unprecedented detail.

As mentioned above, the tools required to utilize this full-field information in the evaluation and calibration of models need further development. As an example, there may be dozens of grains in the ROI, each with a differing material orientation. Even if it is assumed that each grain has the same properties but with differing orientations, correlating the measured full-field behavior with the full-field behavior as predicted by a crystal-plasticity model, for example, is a very complex process. There will be many parameters that need to be determined during this correlation process, requiring high-performance computing, including the effective use of parallel processing. This requirement becomes even greater when *distributions* of parameter values for probabilistic design are desired, as opposed to single-valued parameters.

So, the challenges in this area are immense. However, the potential payoffs are also immense. In fact, it is argued that an approach such as the one described here, is the only approach that can work in many cases. In most models of nonlinear material behavior, there are "too many parameters chasing too few data," and there are severe uniqueness problems in using traditional

methods for evaluating and calibrating these many-degree-of-freedom models. The use of full-field experimental techniques, in connection with high-performance computing resources, makes feasible a new level of model fidelity and detail, since the volume of testing required with the conventional approach is reduced by orders of magnitude.

Approach

Digital Image Correlation (DIC) has become a mature and commercially-viable technology. Much of the experimental and theoretical groundwork in this area was laid in the 1980s and early 1990s [2, 3, 4, 5]. However, using DIC at micro- and nano-scales presents many challenges, and successful, low-strain work using DIC at these scales is relatively uncommon. For DIC, the usual physical challenges in visible-light, high-magnification work are complicated by issues such as vibration from loading systems and subtle spatial distortions in optical lenses. Use of an *in-situ* loading stage in a scanning electron microscope (SEM) is an obvious solution to these issues, but SEM imaging presents its own set of issues, including set-up time and expense and spatial distortions and image drift [6, 7]. For these reasons, the approach in the present work is to use visible-light microscopy, building on previous work in a large-colony intermetallic [1]. The focus of the present work is on nickel-base superalloys with microstructural features of normal size. There are three main aspects to this work: 1) full-field experimental work, 2) high-fidelity modeling of the actual microstructures studied, and 3) the correlation between 1) and 2). The emphases in this paper will be on the first and second areas, but the need for work in the third area is recognized, and efforts in this area are on-going. Two general types of problems are being studied using the same philosophy of acquiring full-field, two-dimensional deformation data and integrating this with advanced, high-fidelity models of actual microstructures. These two types of problems are deformations near features-of-interest (FOIs), which may be cracks, defects, or crack-precursors, and microstructural deformation without the presence of FOIs. By studying the effect of microstructual variability on fatigue-crack precursors and fatigue cracks, we hope to better understand the fundamental physics of fatigue variability.

Full-field Experimental Effort

A similar system to that used in previous work [1] is being used, with the only significant difference being the necessity for higher-magnification in working with superalloys which have much smaller microstructural features than those of the intermetallic studied previously. Figures 3 and 4 show full-field deformation results for an area without FOIs and near a small fatigue crack, respectively. Naturally, it is not possible for a paper of this length to show even a small fraction of the data collected, but the figures do give an idea of the type of data that is being acquired. As noted, the data displayed for Figure 3 is the maximum, in-plane, principal strain mapped over the grain structure. For Figure 4, the left side of each figure shows displacement vectors of exaggerated length superimposed over images of a small, surface, fatigue crack, whereas the right side of each figure shows surface plots of the full-field displacements in each of the two in-plane directions. Since crack-opening and crack-sliding displacements (COD and CSD) are of great interest in crack problems, concentrating on displacements rather than strains is appropriate for this work. The top figure shows the overall displacements, after rigid-body displacements have been removed. For the bottom figure, a linear fit of each of the in-plane displacements is done for all the data, and this fit is algebraically subtracted from the overall data. This enables the study of what is of most interest, the local behavior caused by the crack.

Modeling

As described in the Introduction, the fullest possible integration of the full-field experimental results with high-fidelity models is the goal of this work. To geometrically model the actual microstructure from the experimental results, orientation imaging microscopy (OIM) is used.

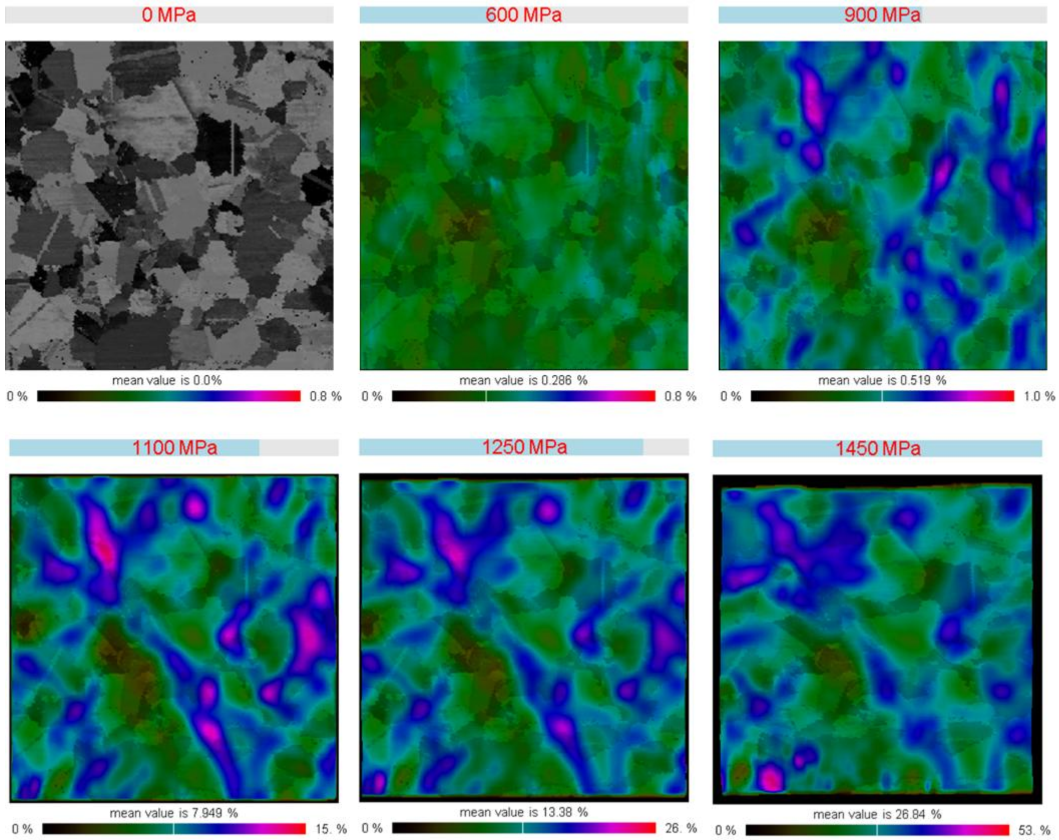

Figure 3. Full-field, in-plane, maximum principal stress in a nickel-based superalloy undergoing tensile loading. Field of view is approximately 300 μm.

Figure 5 shows a typical OIM map for a region near a crack (top), along with a secondary-electron (SE) image of the same crack (bottom). The crack has grown from a defect which is apparent in the SE image.

The OIM process gives the full, three-dimensional orientation of all the grains in the region of interest. The goal is to convert this information into a good, "watertight", finite-element model using a robust, consistent, automated tool. The meaning of "watertight" in this context is that there can be no spatial gaps in the model and no geometric discontinuities, other than the actual physical discontinuities, such as cracks and voids. Since only the orientations of the surface grains are known, a so-called "2½D" model is developed, where the model is three-dimensional and the three-dimensional orientations of the grains are included, but geometrically the grains are prismatic through the thickness of the model. Although the grains are prismatic through the thickness, the crack front can be three-dimensional in shape. Figure 6 shows such a model of the crack region shown in Figure 5, along with an illustration of a typical result from a finite-element analysis of this model. For this illustration, displacements are exaggerated, and the maximum principal strain is the contour variable. Through these types of analyses, the effect of material microstructure on damage evolution can be studied, enabling better understanding of the physics behind variability in damage evolution.

The procedure for uncracked regions is similar. For these regions, the goal is to determine distributions of material parameters through correlation of modeling and experimental full-field results. This calibration process of actual polycrystalline material is key to developing sophisticated models of complicated material behavior. For example, a crystal-plasticity material-behavior model [8, 9, 10] has been incorporated in these geometric models. An example of the

output from such a combination is shown in Figure 7. The effect of varying grain orientations on stress distributions can be studied, also, through a Monte-Carlo-type automated variation of the grain orientations in the model. In fact, the effects on stress distributions on various texturing effects can be incorporated through the automated generation of models with the proper grain-orientation distributions. In this way, instead of so-called "statistically-equivalent" microstructures (in geometric and grain-orientation senses) being used, the most important distribution, which is generally the stress distribution, can be studied and correlated.

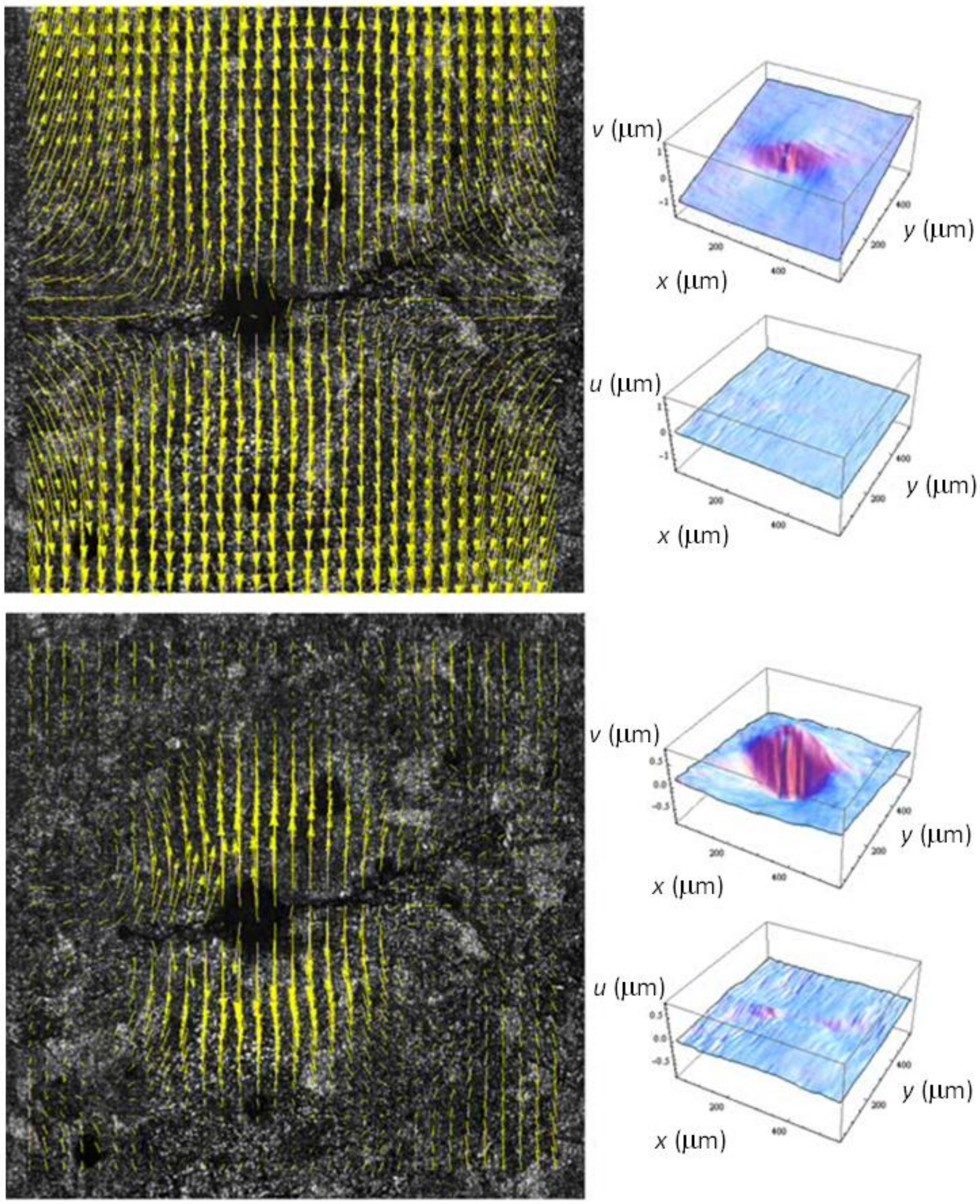

Figure 4. Overall (top) and local (bottom) displacements for a small fatigue crack undergoing tensile loading. Vectors are exaggerated.

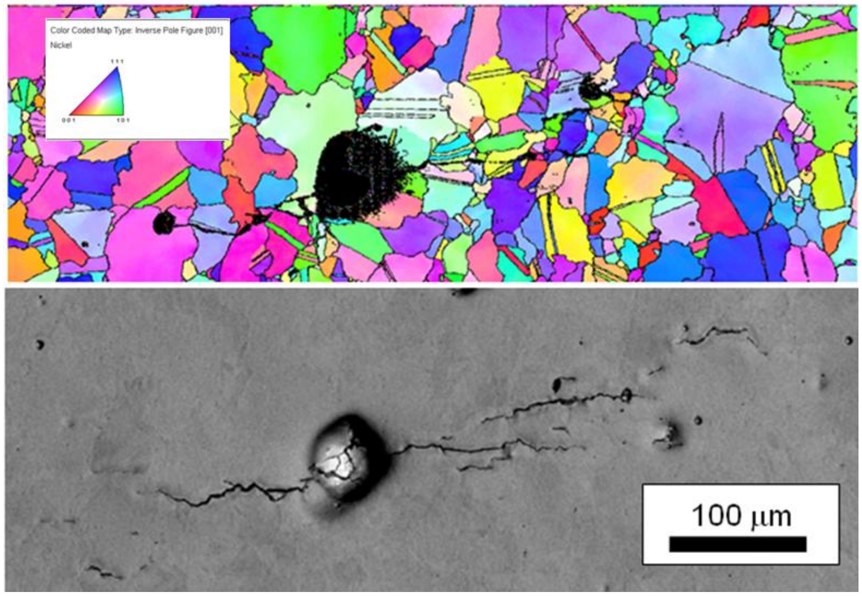

Figure 5. Orientation imaging microscopy (OIM) map (top) and secondary-electron image (bottom) of a region near a fatigue crack in a nickel-based superalloy.

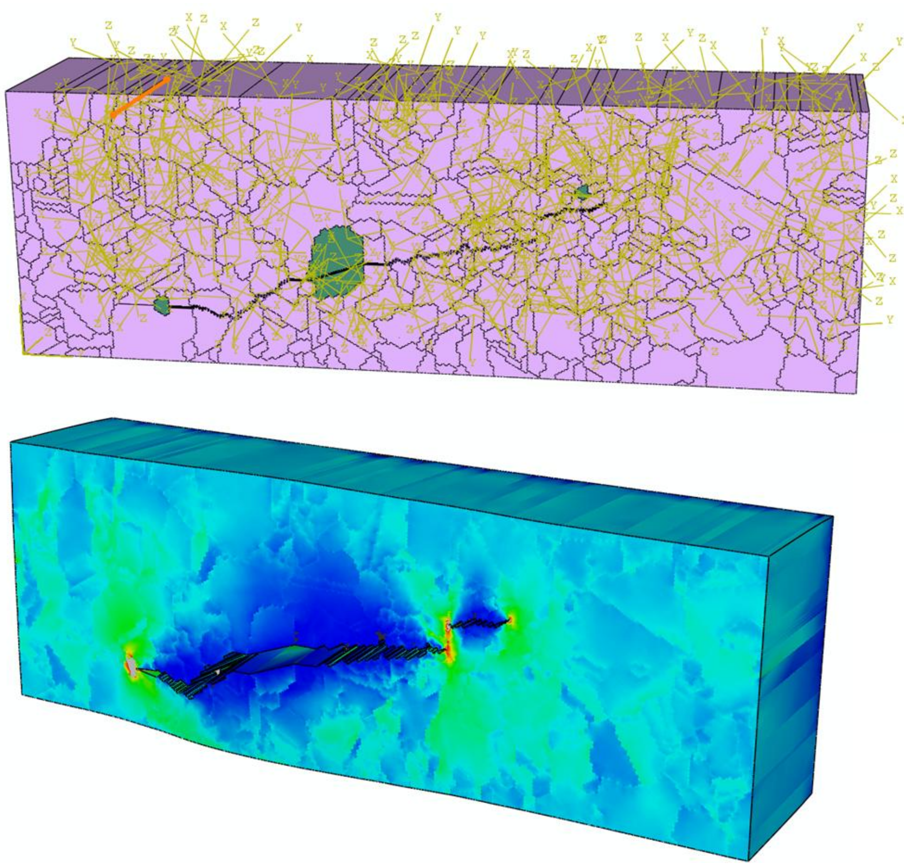

Figure 6. High-fidelity, analysis-ready, model of the crack region (top) and typical finite-element-analysis results (bottom).

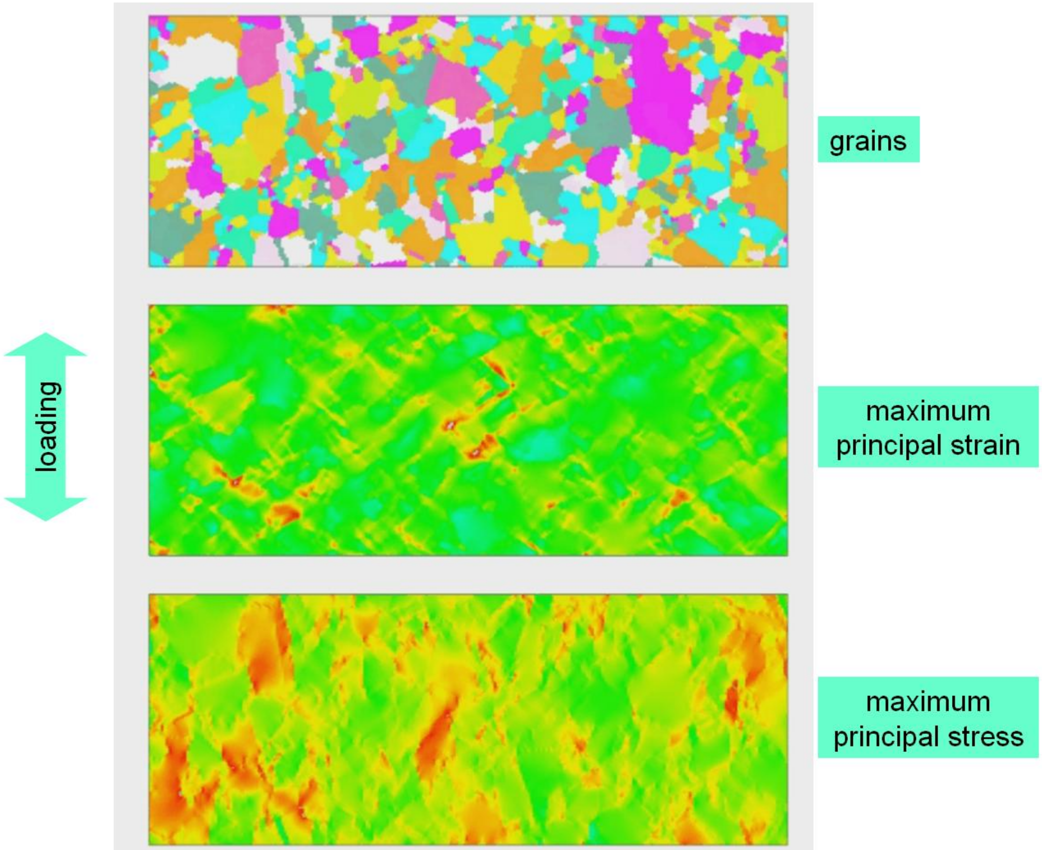

Figure 7. Results from an analysis combining a high-fidelity geometric model of actual material microstructure with a crystal-plasticity model.

Conclusion

Sophisticated tools for both experimental full-field data acquisition and high-fidelity models of actual microstructure have been developed and used in the study of regions of materials with and without damage. These tools can be employed on many other problems at various size scales. The philosophy described in the Introduction also requires the development of sophisticated tools to correlate the experimental and modeling information. In the author's opinion, this is an area for much useful research in both mathematics and engineering. The increasing availability of full-field experimental techniques, which, as described in the Introduction, enables us to move beyond fitting just a few points, also requires new, rigorously developed tools in correlation and calibration of full-field information, especially as we move into three-dimensional techniques.

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